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Supplementary Information

for the article

Magnetostructural relationships in polymorphic ethylmalonate-containing copper(II) coordination polymers

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Table S1. Crystallographic data for complexes **1**-**3**

	1	**2**	**3**
Formula	$C_{10}H_{22}O_{13}Cu_2$	$C_5H_8O_5Cu$	$C_5H_6O_6Cu$
Fw	477.35	211.64	225.64
Crystal system	Orthorhombic	Orthorhombic	Hexagonal
Space group	$C222_1$	$C2cb$	$P6_5$
a (Å)	9.9885(2)	9.770(3)	11.5965(8)
b (Å)	11.9939(2)	9.921(3	-
c (Å)	14.1518(3)	14.477(3)	10.5437(6)
V (Å)	1695.40(6)	1403.2(7)	1227.94(14)
Z	4	8	6
T (K)	293(2)	293(2)	293(2)
ρ_{calc} (g·cm^{-3})	1.870	1.985	1.831
μ (Mo Kα, mm^{-1})	2.574	3.081	2.656
λ (Mo Kα, Å)	0.71073	0.71073	0.71073
Index ranges	$-14 < h < 14$	$-12 < h < 10$	$-15 < h < 13$
	$-17 < k < 17$	$-10 < k < 12$	$-15 < k < 15$
	$-20 < l < 20$	$-18 < k < 15$	$-13 < l < 9$
Indep. Reflections (R_{int})	2801 (0.0286)	1408 (0.0653)	1916 (0.0440)
Obs. Reflections [$I > 2\sigma(I)$]	2706	1058	1813
Flack Parameter	0.005(13)	0.52(4)	0.03(4)
Parameters	135	108	120
Goodness of fit	1.053	1.030	1.159
R [$I > 2\sigma(I)$]	0.0213	0.0458	0.0509
R_w [$I > 2\sigma(I)$]	0.0489	0.0894	0.1333
R (all data)	0.0225	0.0759	0.0558
R_w (all data)	0.0494	0.0980	0.1356

Table S2. Selected bond lengths (Å) and angles (º) for complexes **1**-**3** [a]

		1	
Cu(1)–O(2)	2.0209(15)	Cu(2)–O(2w)	1.9727(17)
Cu(1)–O(4)	1.9477(14)	Cu(2)–O(3w)	1.9700(17)
Cu(1)–O(1w)	1.999(2)	Cu(2)–O(1)	2.3936(14)
O(2)–Cu(1)–O(4)	90.87(6)	O(2w)–Cu(2)–O(3w)	174.35(8)
O(2)–Cu(1)–O(2a)	115.07(10)	O(2w)–Cu(2)–O(1)	88.43(7)
O(2)–Cu(1)–O(1w)	122.46(5)	O(2w)–Cu(2)–O(3wb)	92.55(8)
O(2)–Cu(1)–O(4a)	92.35(7)	O(2w)–Cu(2)–O(1b)	91.04(7)
O(4)–Cu(1)–O(1w)	87.00(5)	O(2w)–Cu(2)–O(2wb)	84.65(11)
O(4)–Cu(1)–O(4a)	174.01(10)	O(3w)–Cu(2)–O(1)	96.54(7)
		O(3w)–Cu(2)–O(1b)	83.96(7)
		2	
Cu(1)–O(2)	1.947(5)	O(2)–Cu(1)–O(1w)	96.5(3)
Cu(1)–O(4)	1.956(6)	O(4)–Cu(1)–O(1c)	86.3(3)
Cu(1)–O(1c)	1.963(6)	O(4)–Cu(1)–O(3d)	85.2(3)
Cu(1)–O(3d)	1.972(6)	O(4)–Cu(1)–O(1w)	94.0(3)
Cu(1)–O(1w)	2.264(7)	O(1c)–Cu(1)–O(3d)	92.7(3)
O(2)–Cu(1)–O(4)	89.8(3)	O(1c)–Cu(1)–O(1w)	102.0(3)
O(2)–Cu(1)–O(1c)	161.3(3)	O(3d)–Cu(1)–O(1w)	104.2(2)
O(2)–Cu(1)–O(3d)	85.2(3)		
		3	
Cu(1)–O(1e)	1.977(5)	O(1e)–Cu(1)–O(1w)	92.1(3)
Cu(1)–O(2)	1.974(5)	O(2)–Cu(1)–O(3f)	89.2(2)
Cu(1)–O(3f)	1.948(5)	O(2)–Cu(1)–O(4)	90.9(2)
Cu(1)–O(4)	1.954(5)	O(2)–Cu(1)–O(1w)	105.7(3)
Cu(1)–O(1w)	2.313(8)	O(3f)–Cu(1)–O(4)	179.8(3)
O(1e)–Cu(1)–O(2)	161.9(2)	O(3f)–Cu(1)–O(1w)	95.5(2)
O(1e)–Cu(1)–O(3f)	92.1(2)	O(4)–Cu(1)–O(1w)	84.6(3)
O(1e)–Cu(1)–O(4)	87.7(2)		

[a] Symmetry codes: (a) = -*x*+1, *y*, -*z*+3/2; (b) = *x*, -*y*+1, -*z*+1; (c) = *x*, *y*-1/2, -*z*+1/2; (d) = *x*+1/2, *y*, -*z*+1/2; (e) -*y*+1, *x*-*y*+1, *z*-1/3; (f) = *y*-1, -*x*+*y*, *z*+1/6.

Table S3. Relevant hydrogen bonds for complexes **1**-**2**[a]

1			
H-bond	*D···A* / Å	*H···A* / Å	*D–H···A* / °
O(1W)–H···O(1g)	2.681(2)	2.06(2)	168(3)
O(2W)–H···O(3h)	2.668(2)	1.93(3)	172(4)
O(2W)–H···O(2b)	2.664(2)	1.97(3)	161(3)
O(3W)–H···O(3i)	2.707(2)	2.09(3)	163(3)
O(3W)–H···O(4j)	2.789(2)	2.02(3)	170(3)
C(2)–H···O(1Wk)	3.484(2)	2.69(3)	132(2)
C(4)–H···O(2a)	3.334(2)	2.36(3)	161.5(18)
2			
H-bond	*D···A* / Å	*H···A* / Å	*D–H···A* / °
O(1W)–H···O(2c)	2.748(8)	1.96(8)	134(3)
O(1W)–H···O(1d)	2.762(7)	1.90(9)	142(6)
C(2)–H···O(1W)	3.278(9)	2.49(8)	138(3)

[a] Symmetry codes: (a) = -*x*+2, *y*, -*z*+3/2; (b) = *x*, -*y*+1, -*z*+2; (c) = *x*, *y*-1/2, -*z*+3/2; (d) = *x*-1/2, *y*, -*z*+3/2; (g) = -*x*+3/2, *y*-1/2, -*z*+3/2; (h) = -*x*+3/2, *y*+1/2, -*z*+3/2; (i) = -*x*+1, *y*, -*z*+3/2; (j) = -*x*+3/2, -*y*+1/2, *z*+1/2; (k) = *x*-1/2, *y*+1/2, *z*.

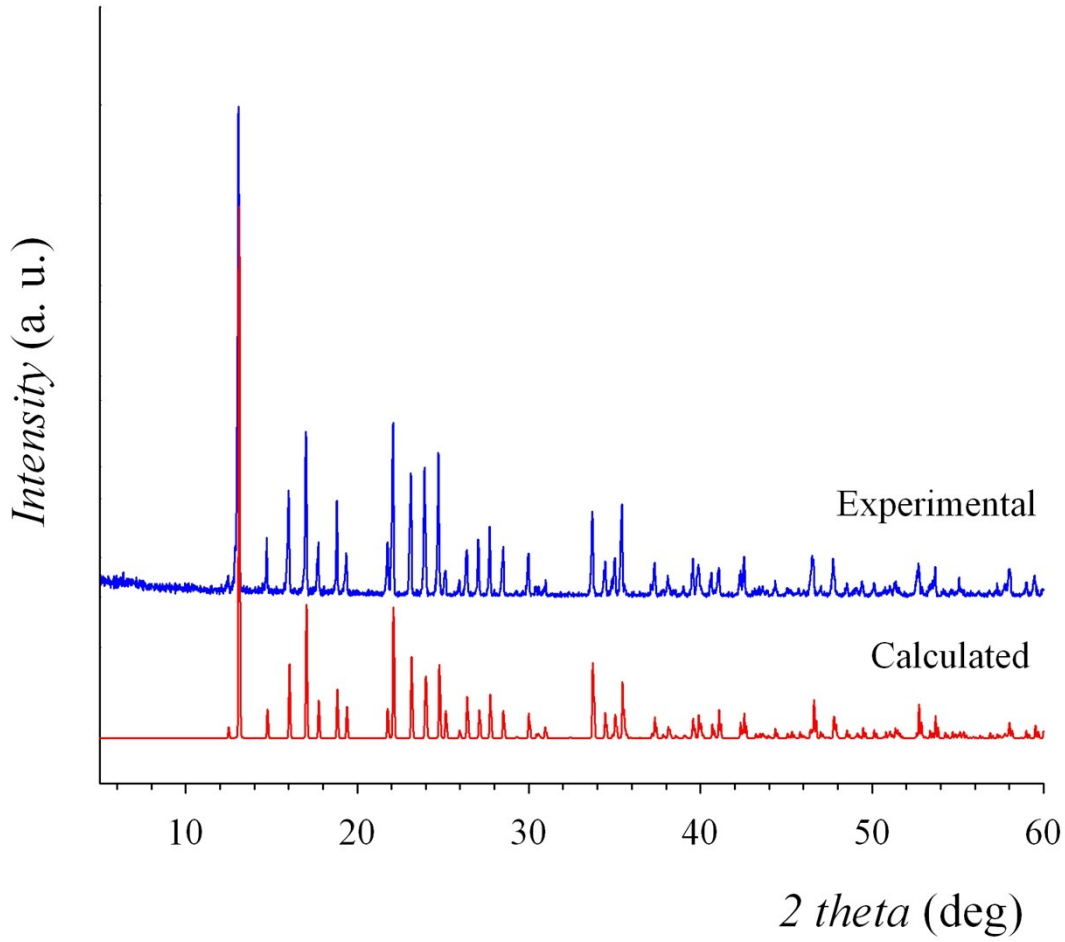


Figure S1. Powder X-ray diffraction pattern for compound **1**.

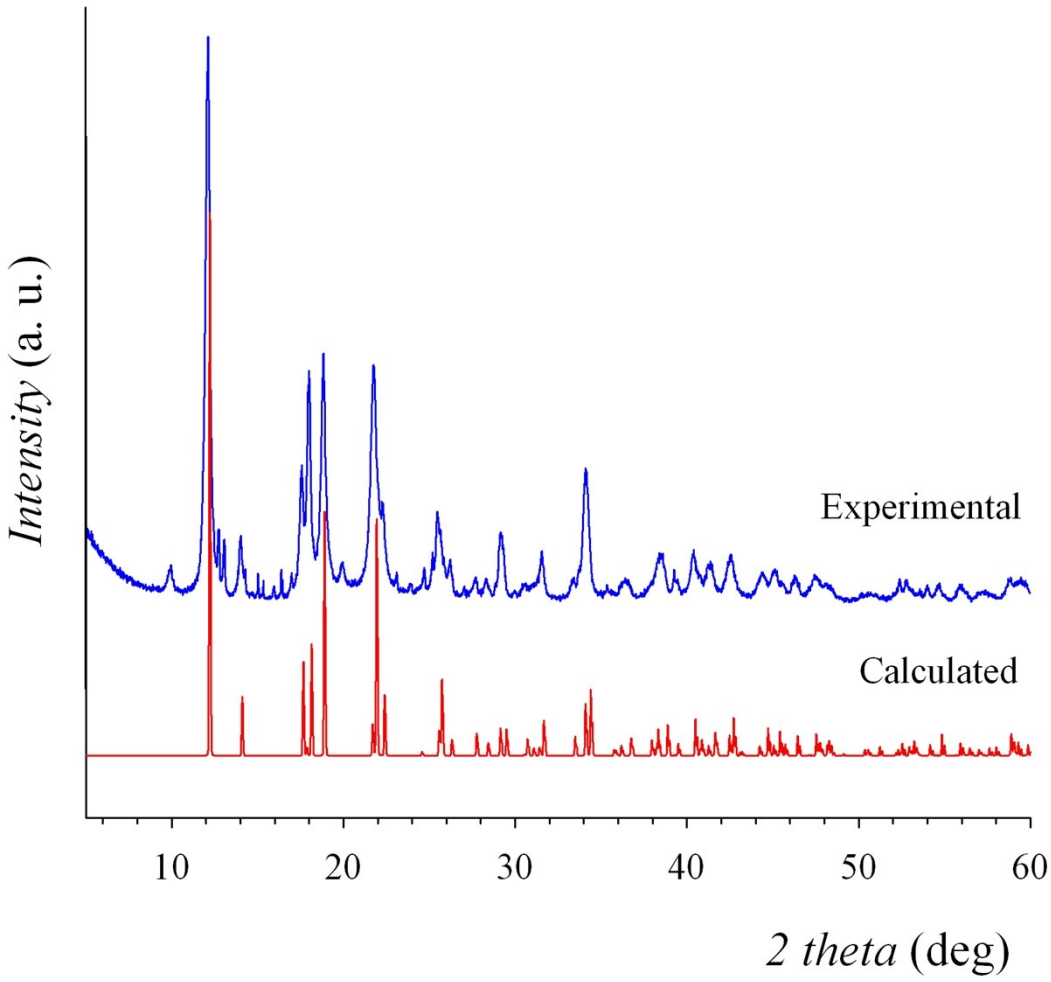


Figure S2. Powder X-ray diffraction pattern for compound **2**.

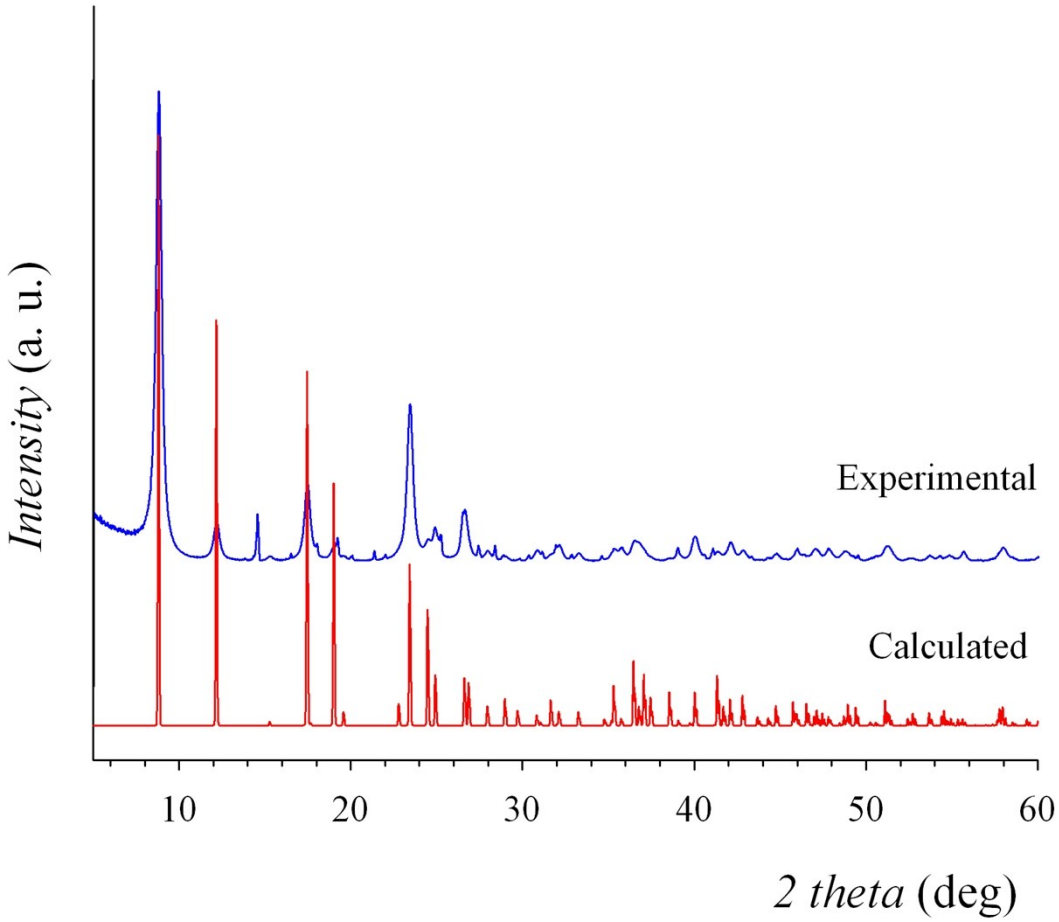


Figure S3. Powder X-ray diffraction pattern for compound **3**.

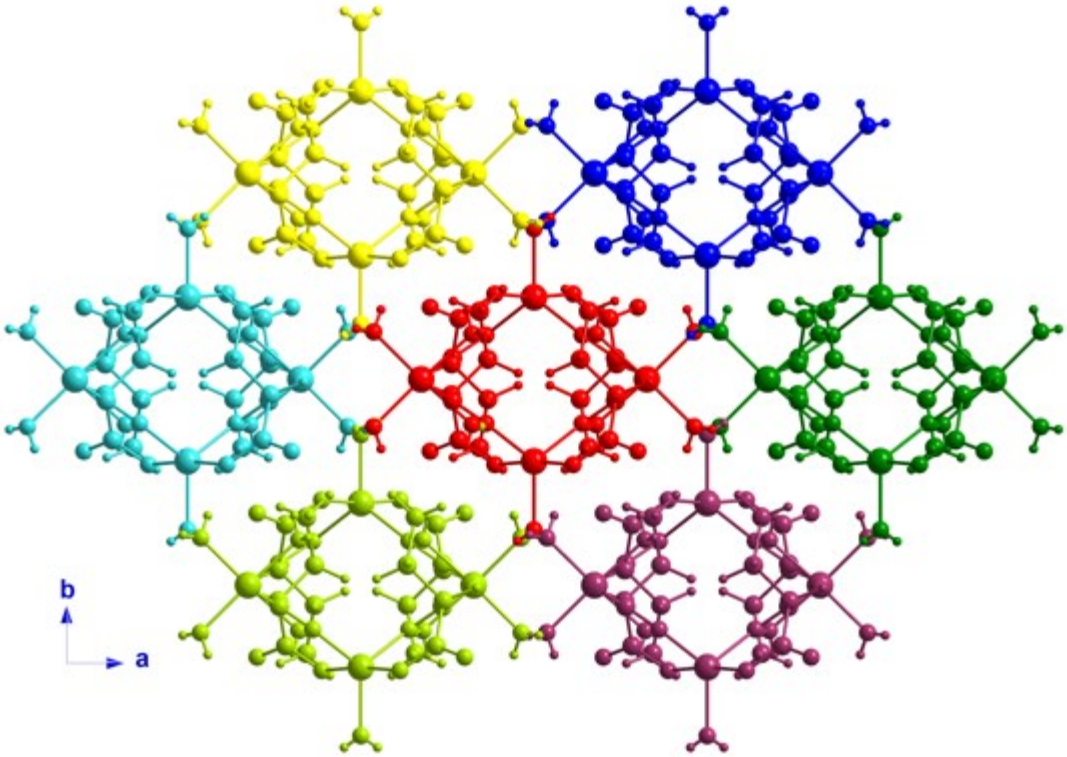


Figure S4. View along the *c* crystallographic axis of the crystal packing of the chain compound **1**. Each $\{[Cu(H_2O)_4][Cu(Etmal)_2(H_2O)]\}_n$ chain is depicted in a different colour.

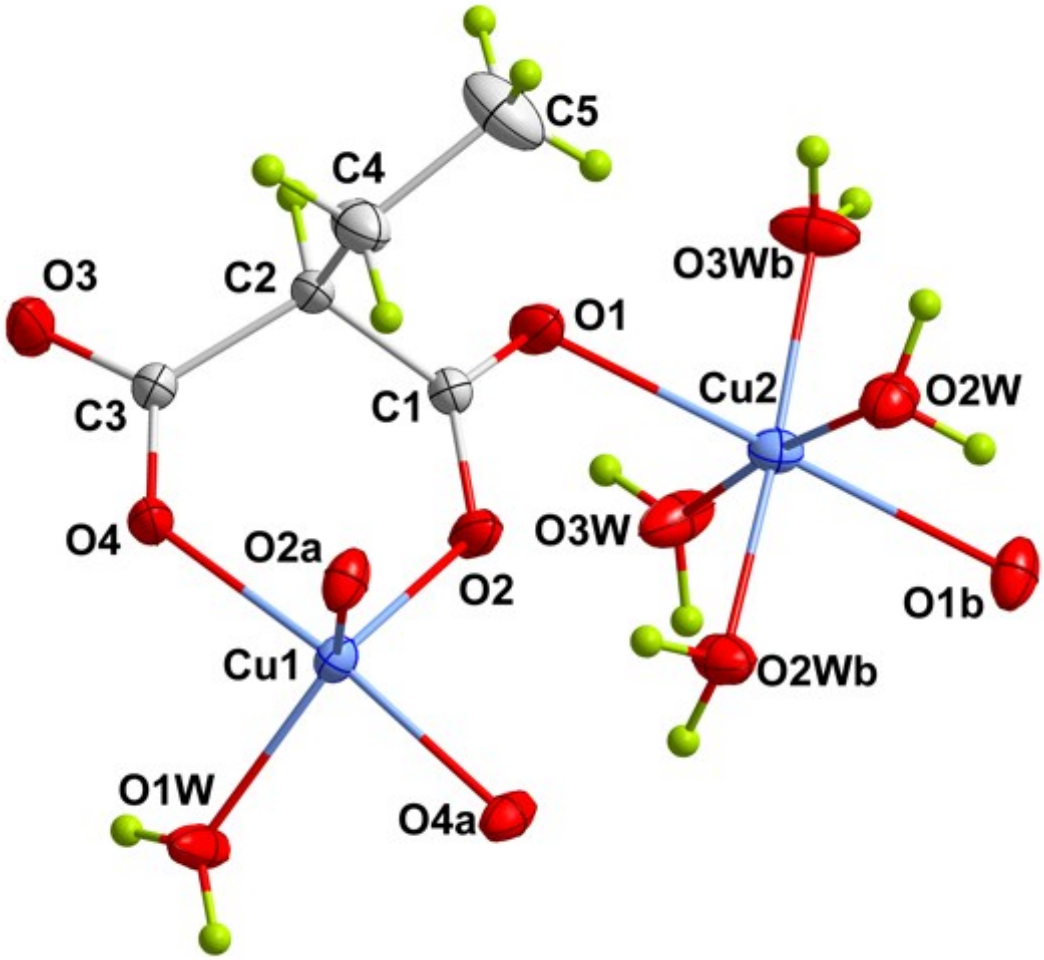


Figure S5. Fragment of the crystal structure of **1** with the atom numbering. The ellipsoids are presented in 50% probability.

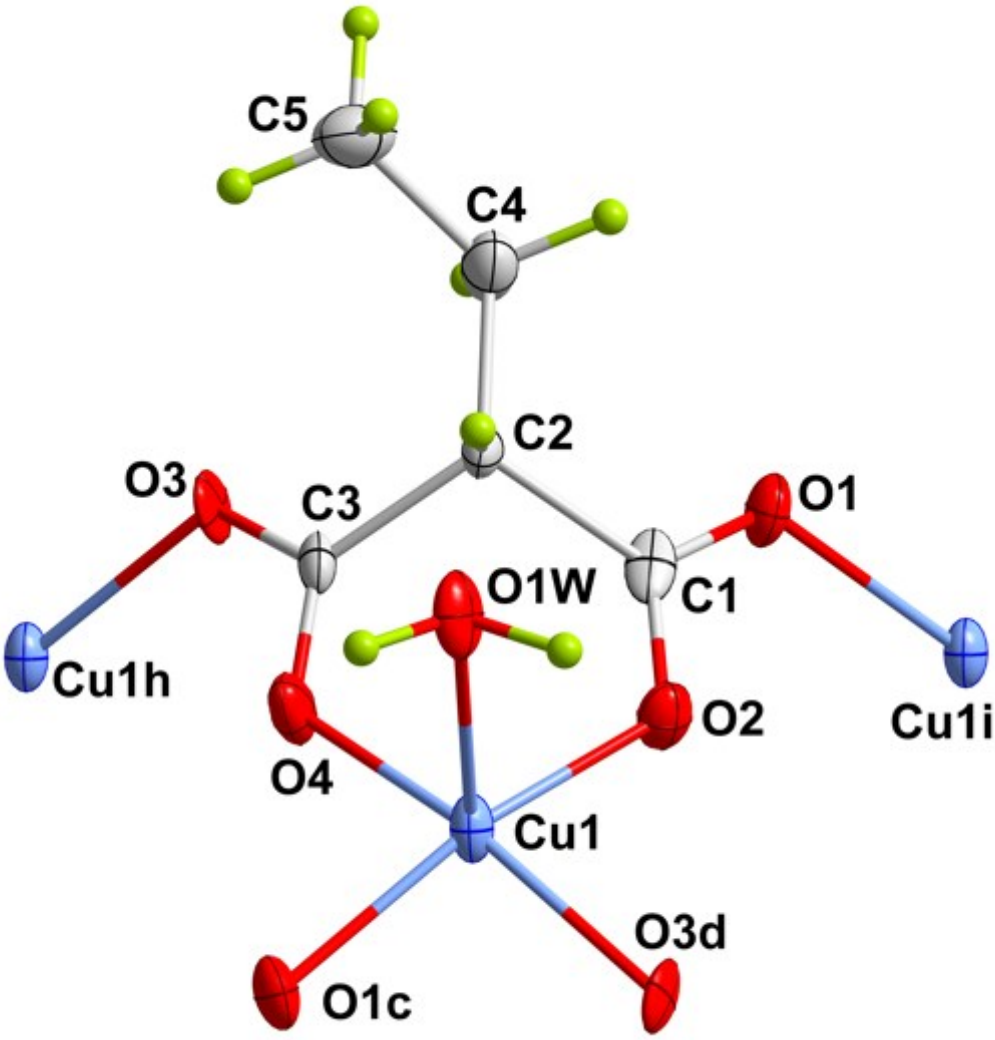


Figure S6. Fragment of the crystal structure of **2** with the atom numbering. Ellipsoids are represented in 50% probability.

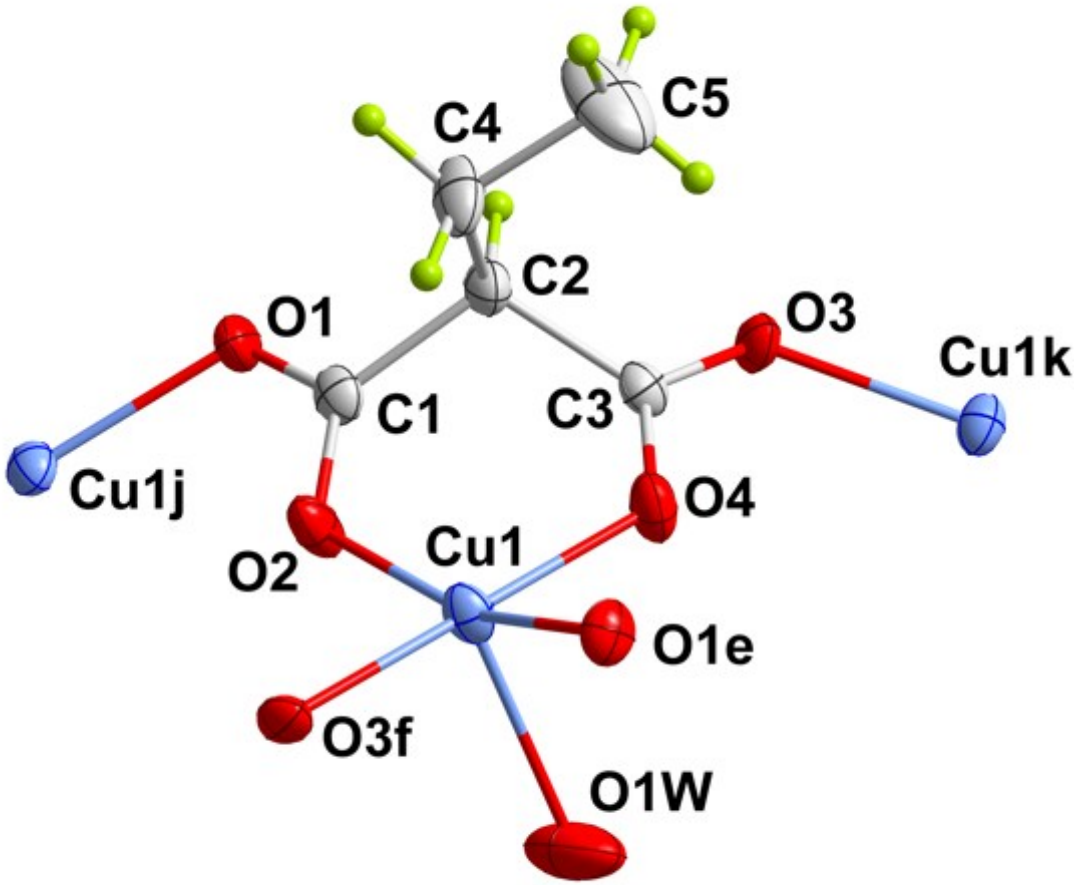
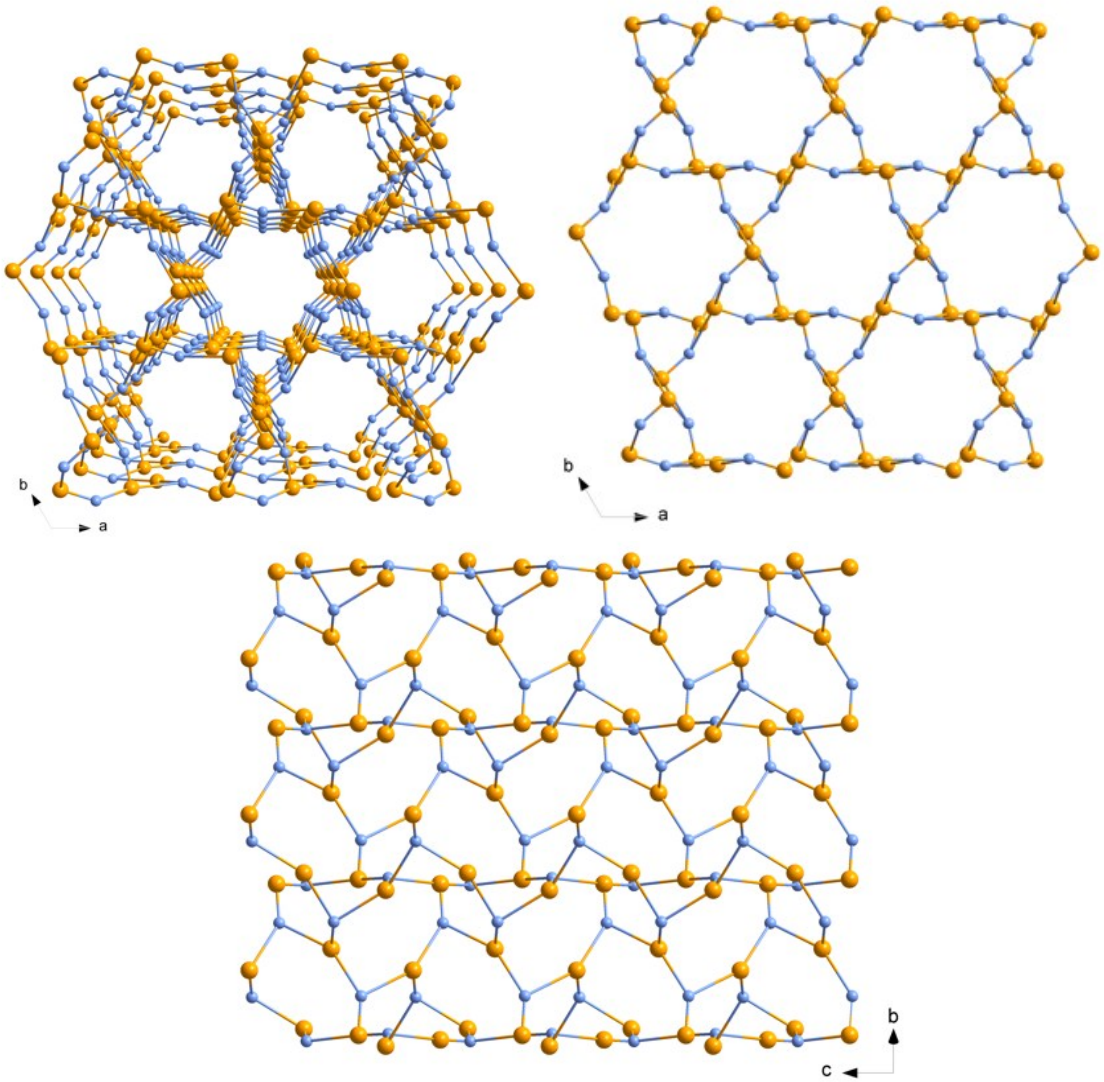


Figure S7. Fragment of the crystal structure of **3** with the atom numbering. Ellipsoids are represented in 50% probability.



Figures S8. Views of the topological representation of the (8,3)-**etd** structure of **3** along the *c* axis (top right), with central projection (top left) and along the *a* axis (bottom). The blue spheres represent the copper(II) ions and the orange ones the $Etmal^{2-}$ ligands.